CCMT

Center For Compressible Multiphase Turbulence Overview

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DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA ·

NNSA

Outline

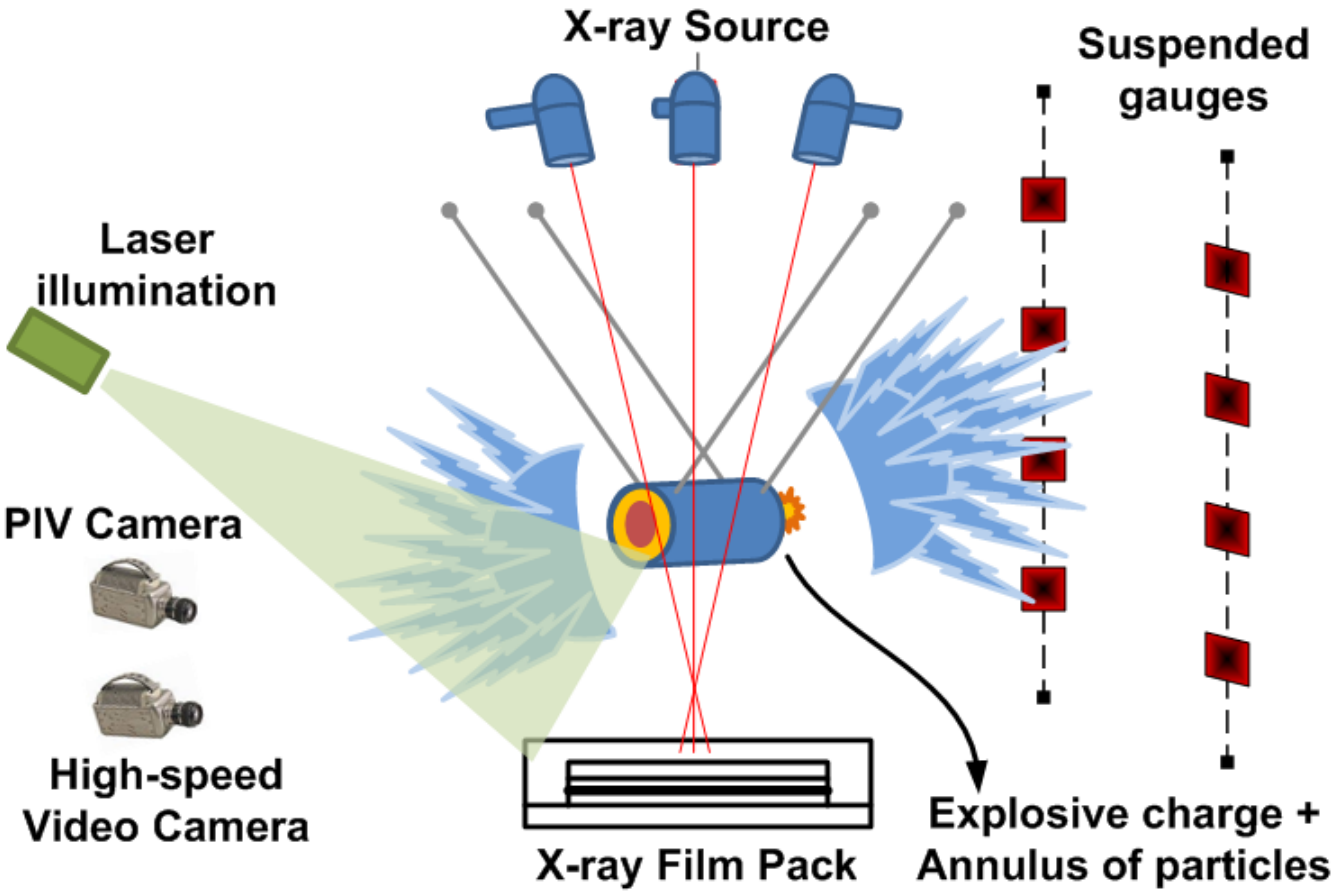
- Demonstration Problem
- Unique Multiscale Approach
- Software Plan
- Exascale Emulation
- V&V, UQ Innovations
- UF Team & Partnership
- NNSA Interaction

Center for Compressible Multiphase Turbulence

Purpose of the Center

- To radically advance the field of CMT
- To advance predictive simulation science on current and near-future platforms with uncertainty budget as backbone
- To advance a co-design strategy that combines exascale emulation, exascale algorithms, exascale CS
- To educate students and postdocs in exascale simulation science and place them at NNSA laboratories

Demonstration Problem



- Integrated simulations
- Experimental measurements for validation

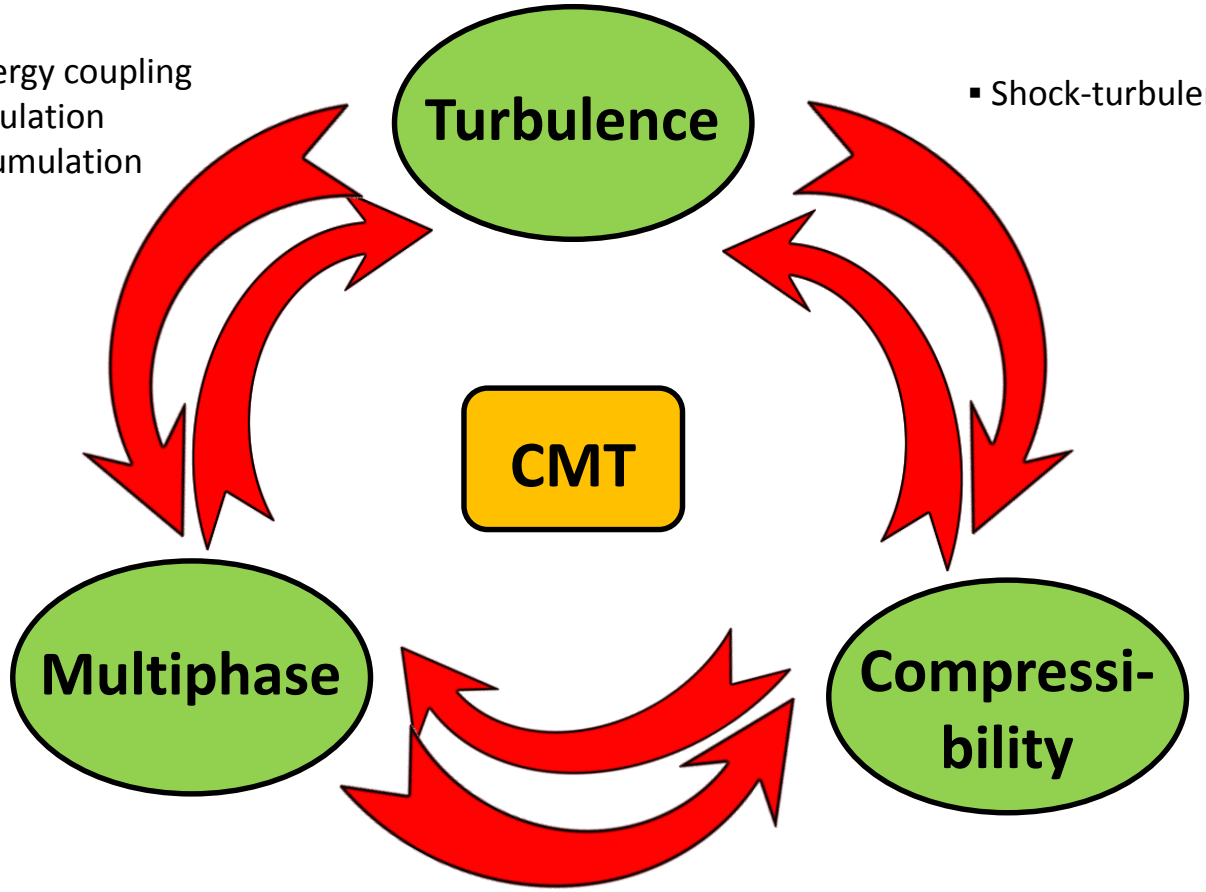
Extreme Multiphase Flow

We desire to perform predictive simulation of these flows with as much multi-scale physics as possible

Single Discipline, But Multi-Physics

Complex interactions require a unified approach

- Momentum, energy coupling
- Turbulence modulation
- Preferential accumulation



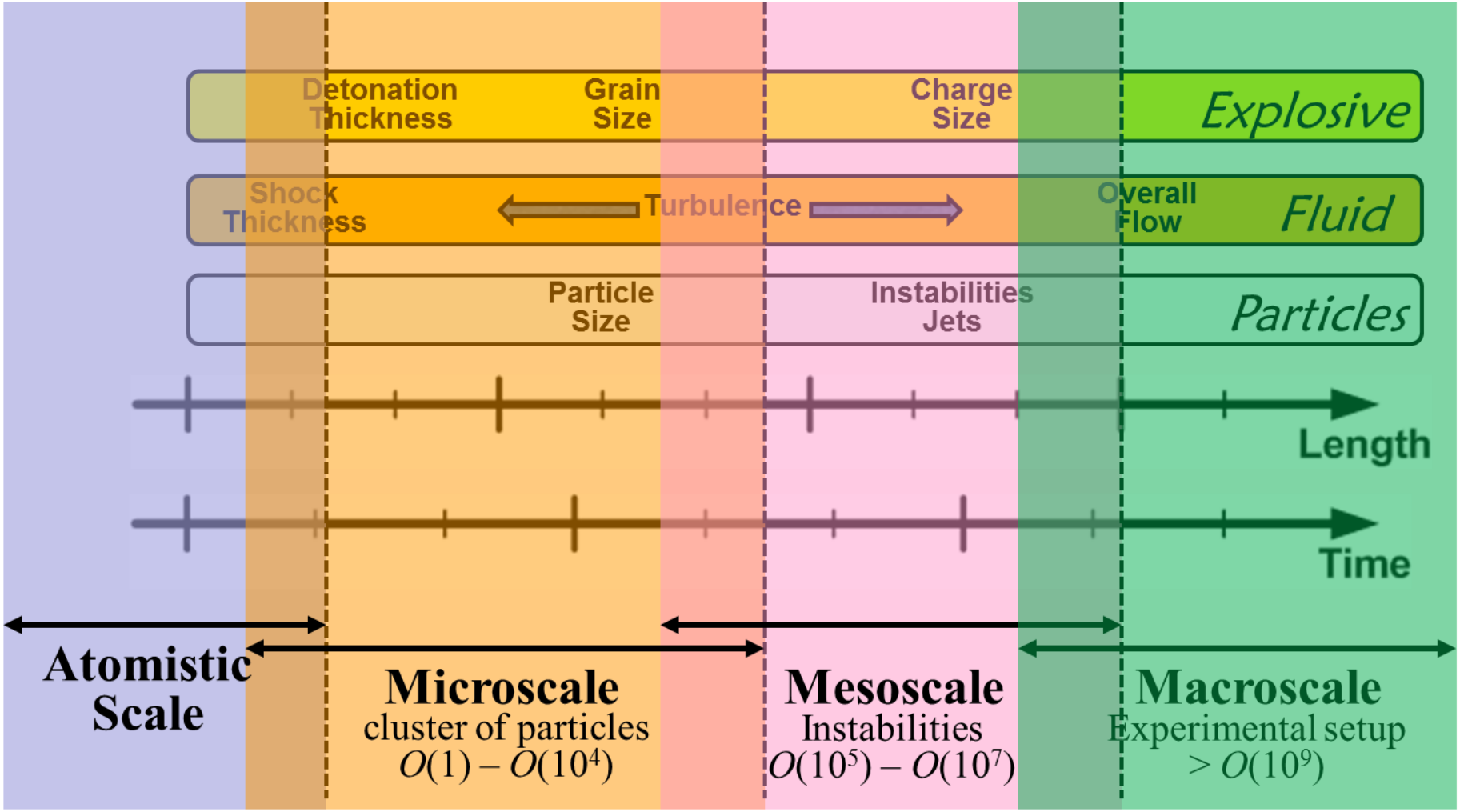
- Shock-turbulence interaction

- Shock-particle interaction
- Additional shocks and expansions
- Strong flow modification

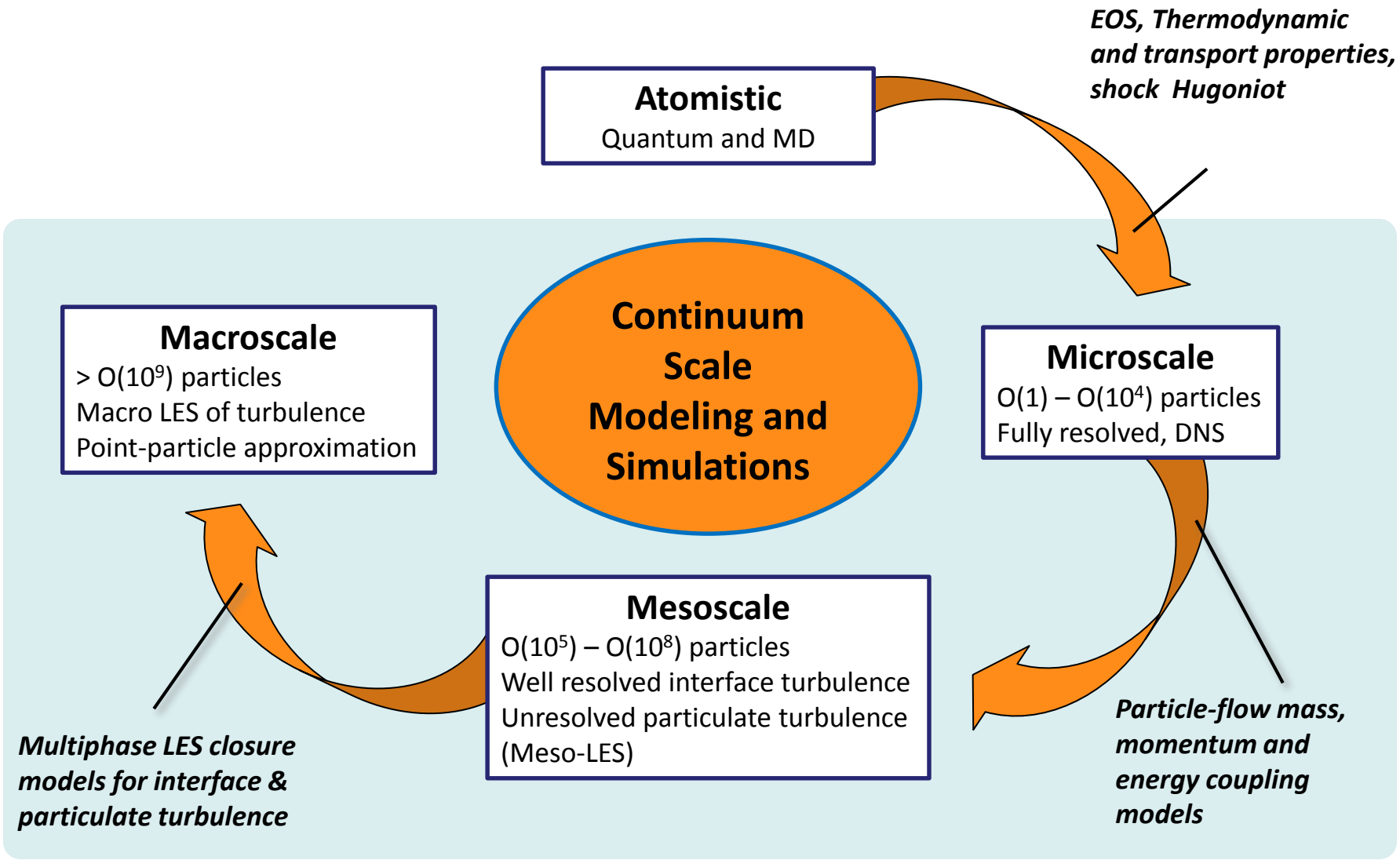
Compressible Multiphase Turbulence

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities induced turbulence
  - Multiphase instability and particulate mixing at the front
  - Self-assemble of explosive-driven particles
- We will minimize the following complications
  - Free-shear and wall turbulence (stay away from boundaries)
  - Detonation physics (use simple, well-studied explosives)
  - Fragmentation or atomization physics (avoid casing, liquids)
  - Reactive physics (use non-reactive metal particles)

Multiscale Approach



Multiscale Coupling Strategy



Multiscale Coupling Strategy

- Our approach is similar in spirit to many ongoing multiscale efforts
  - "Divide, Bridge, and Conquer" strategy
- Unique aspects of present approach
  - Lagrangian particles preserve heterogeneity and anisotropy
  - Opportunities for concurrent macro, meso and microscale simulations
    - But there is no dimensionality reduction as in contact-line problems

Scientific Issues to be Addressed

At Micro to Mesoscale

- Mass, momentum and energy coupling at extreme conditions of pressure and temperature
- Understand and modeling of particle-particle, wake-particle and wake-wake interactions

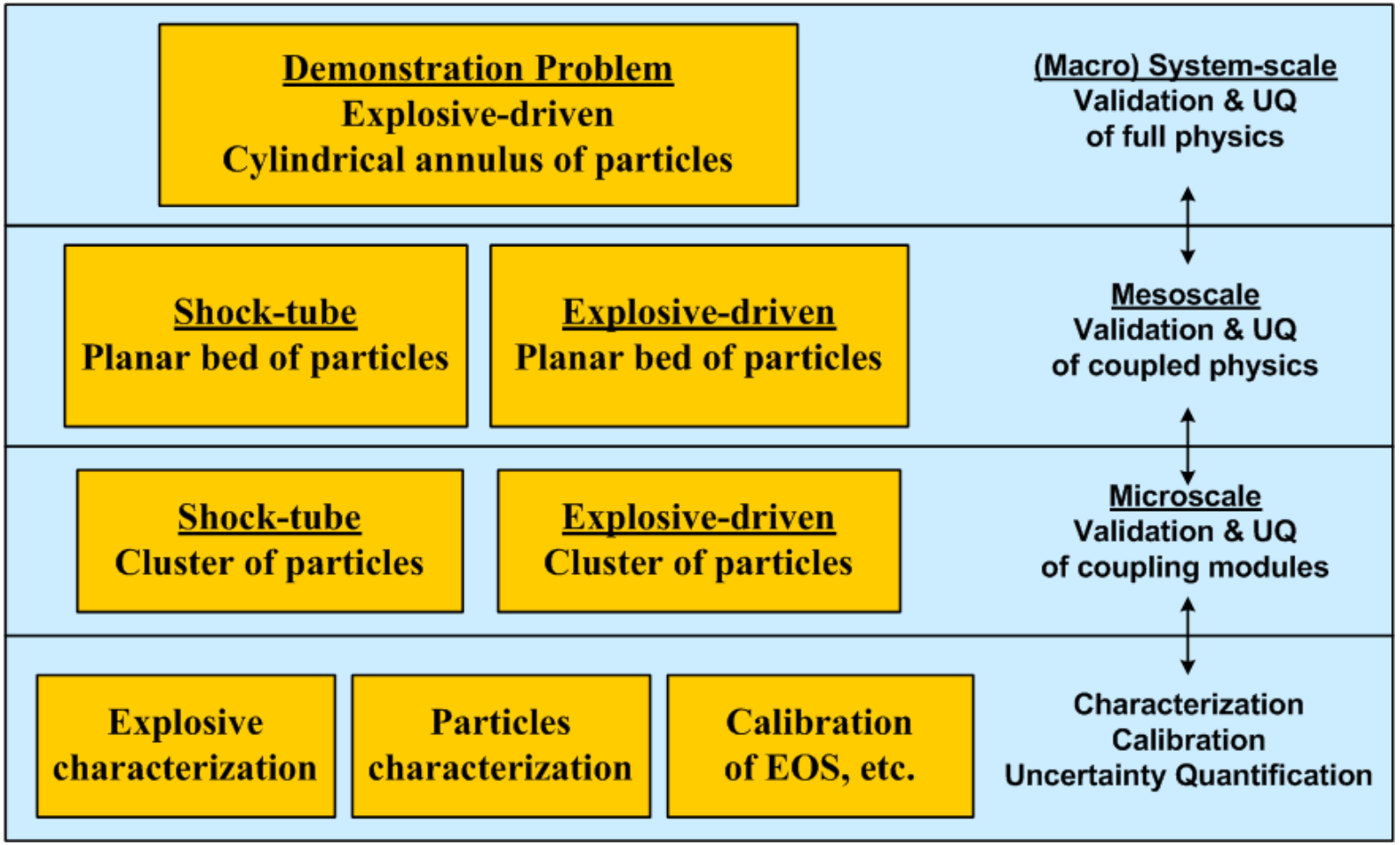
At Meso to Macroscale

- Extend understanding of Rayleigh-Taylor and Richtmeyer-Meshkov instabilities to multiphase flows
- Establish the statistical properties of the interfacial multiphase turbulence
- Physics of particle self-assembly into focused jets

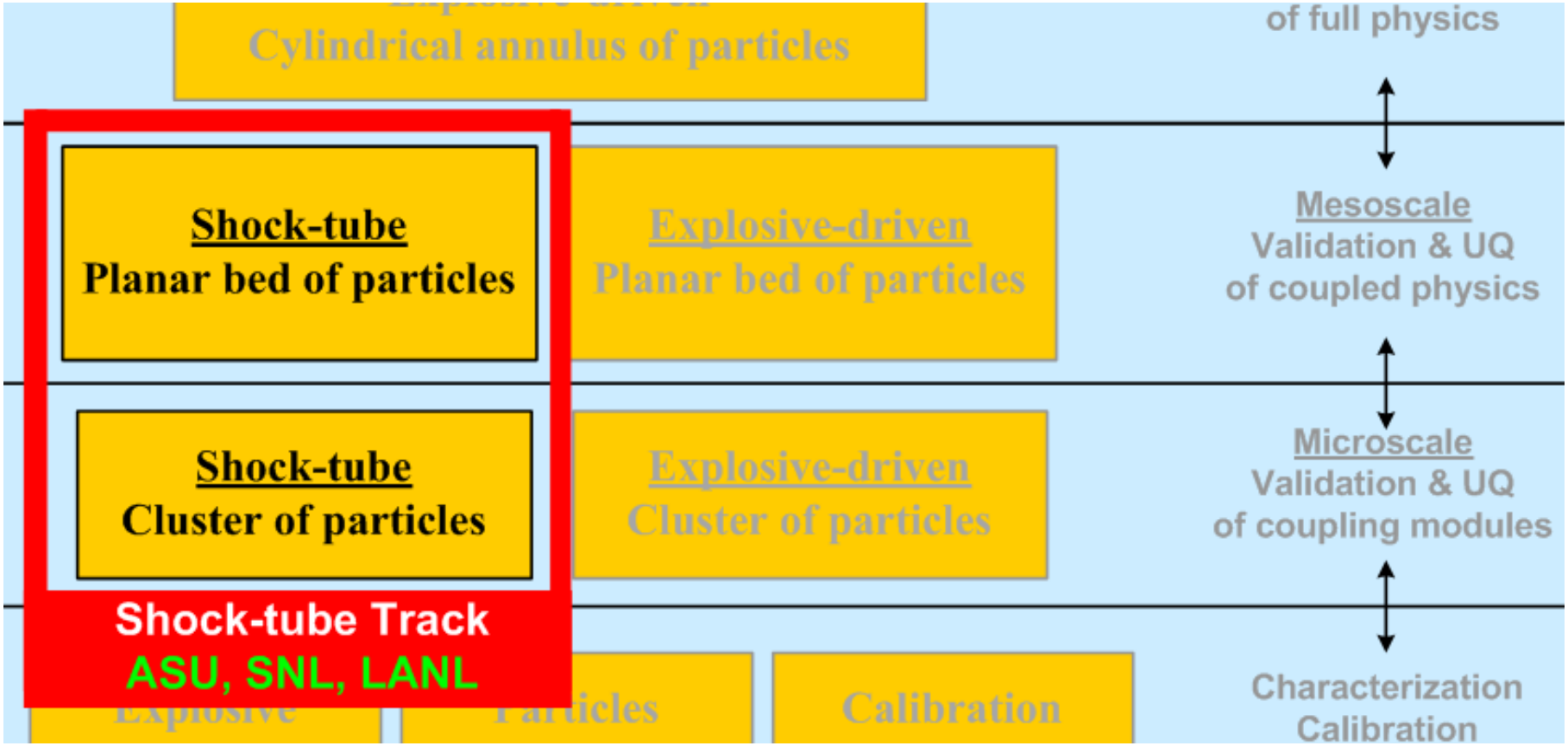
Master Plan

- **Problem Hierarchy:** to systematically validate our multiscale framework and establish uncertainties
- **Systems Engineering Plan:** to build on existing codes and simulation framework for current petascale and future exascale capability
- **Simulation Road Map:** that organizes the proposed integrated simulations and work towards exascale

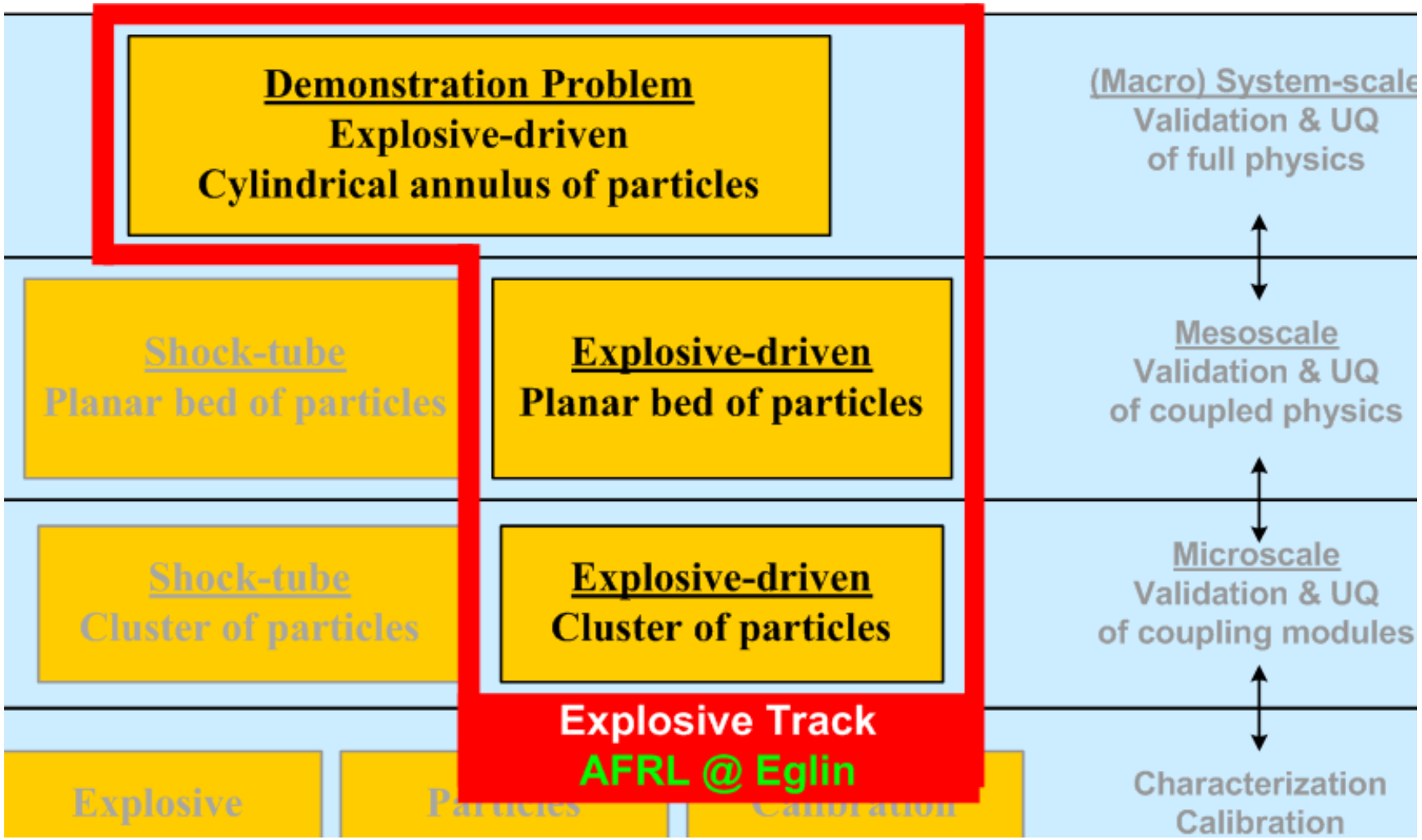
Multi-scale Problem Hierarchy



Multiscale Problem Hierarchy

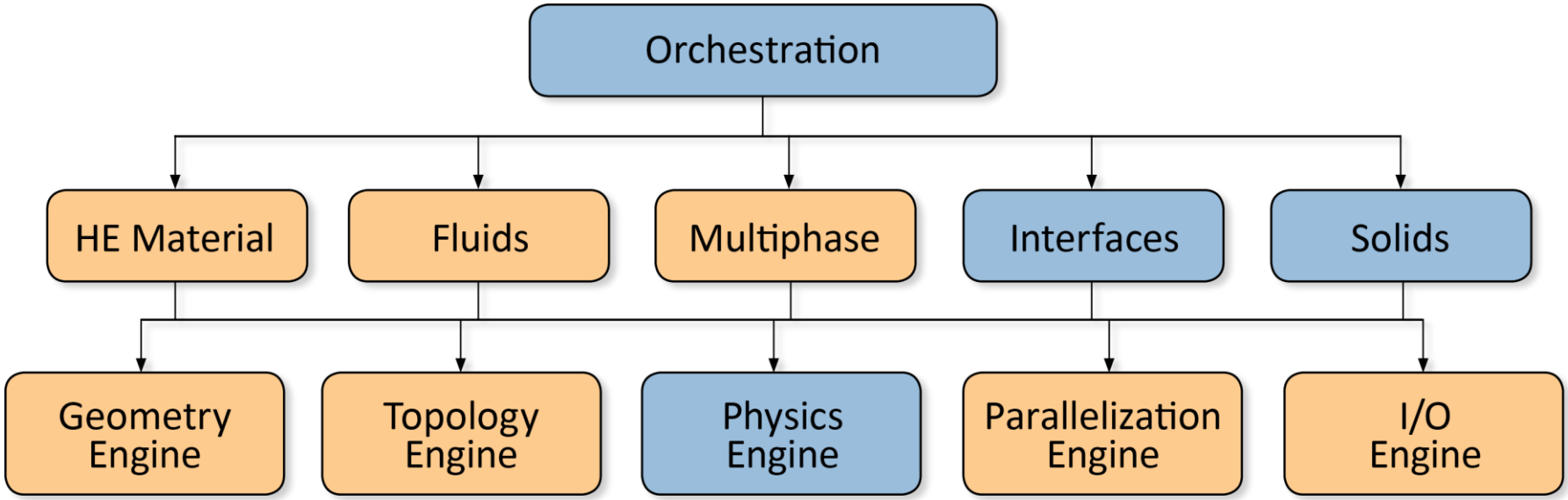


Multiscale Problem Hierarchy



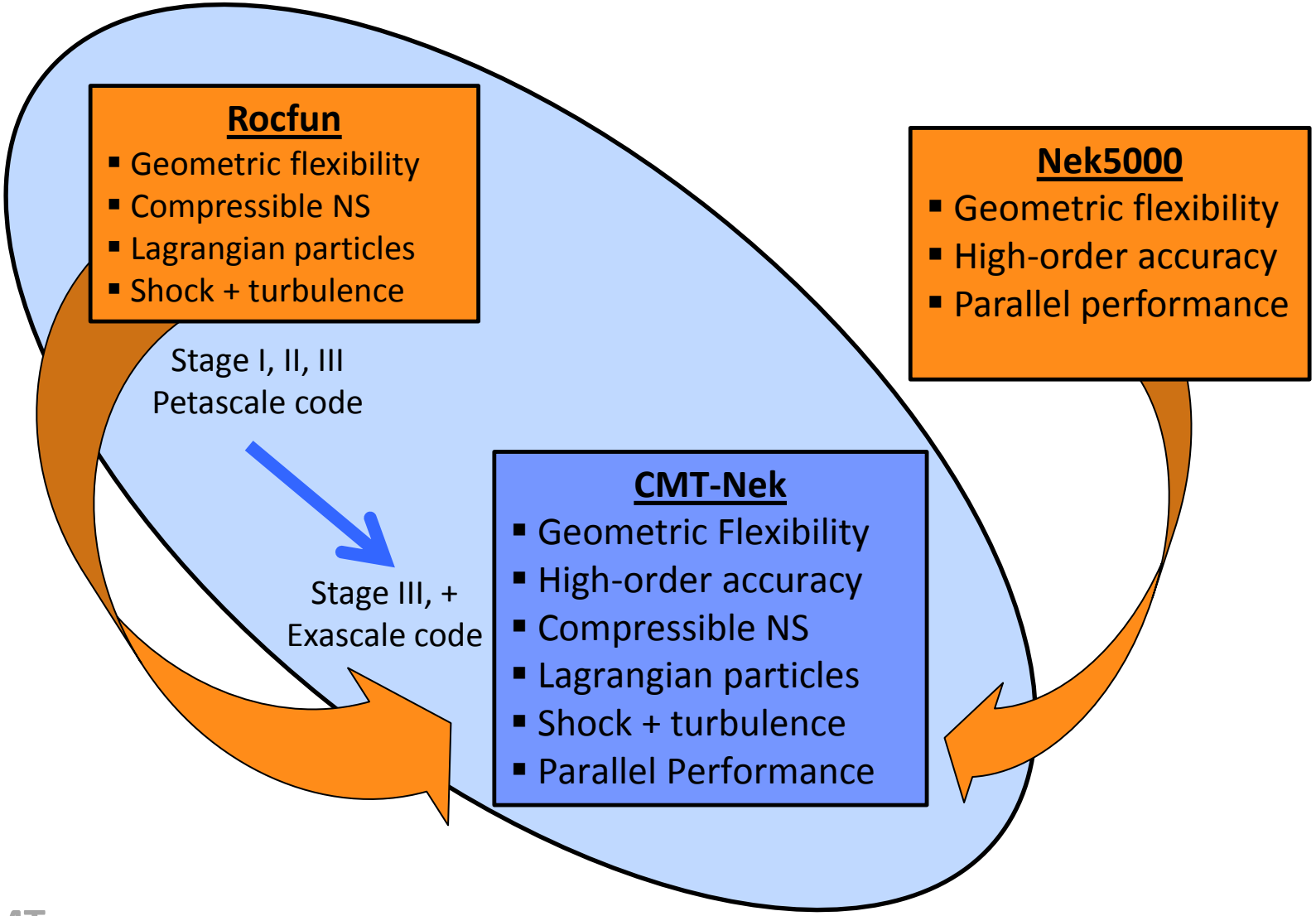
Simulation Roadmap

Rocfun – Existing Integrated Code



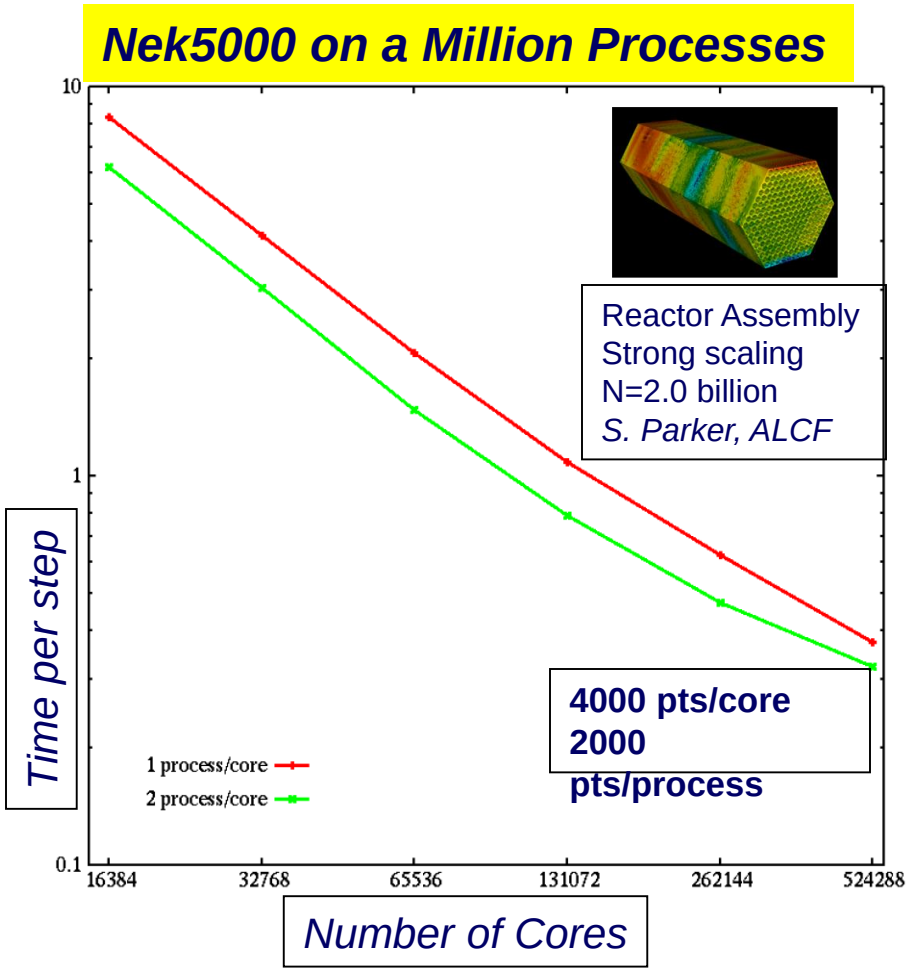
- Developed under ASAP program & continued at University of Florida
- Mature code, used in several projects, demonstrated scalability
- Unified code for *microscale*, *mesoscale* and *macroscale* simulations
- Extensively verified, detailed documentation, rigorous validation

Co-design: Rocfun + Nek5000 = CMT-Nek



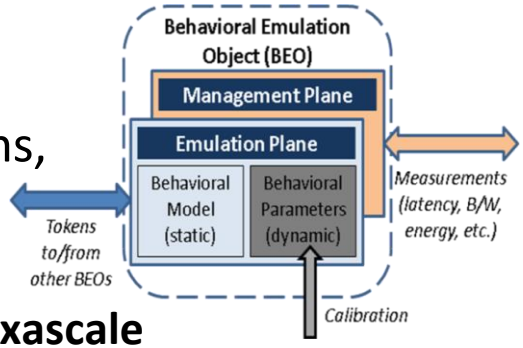
Scalability to Million Processes

- Scales beyond 1 million MPI processes:
  - 524288 cores
    - *1 or 2 ranks / core*
  - 60% parallel efficiency at 1 million processes
  - Scalable multigrid solvers:
    - *15 iterations/step*
  - Scalable I/O: 72 GB/sec



Exascale Emulation with FPGAs

Multiscale approach to Exascale studies:

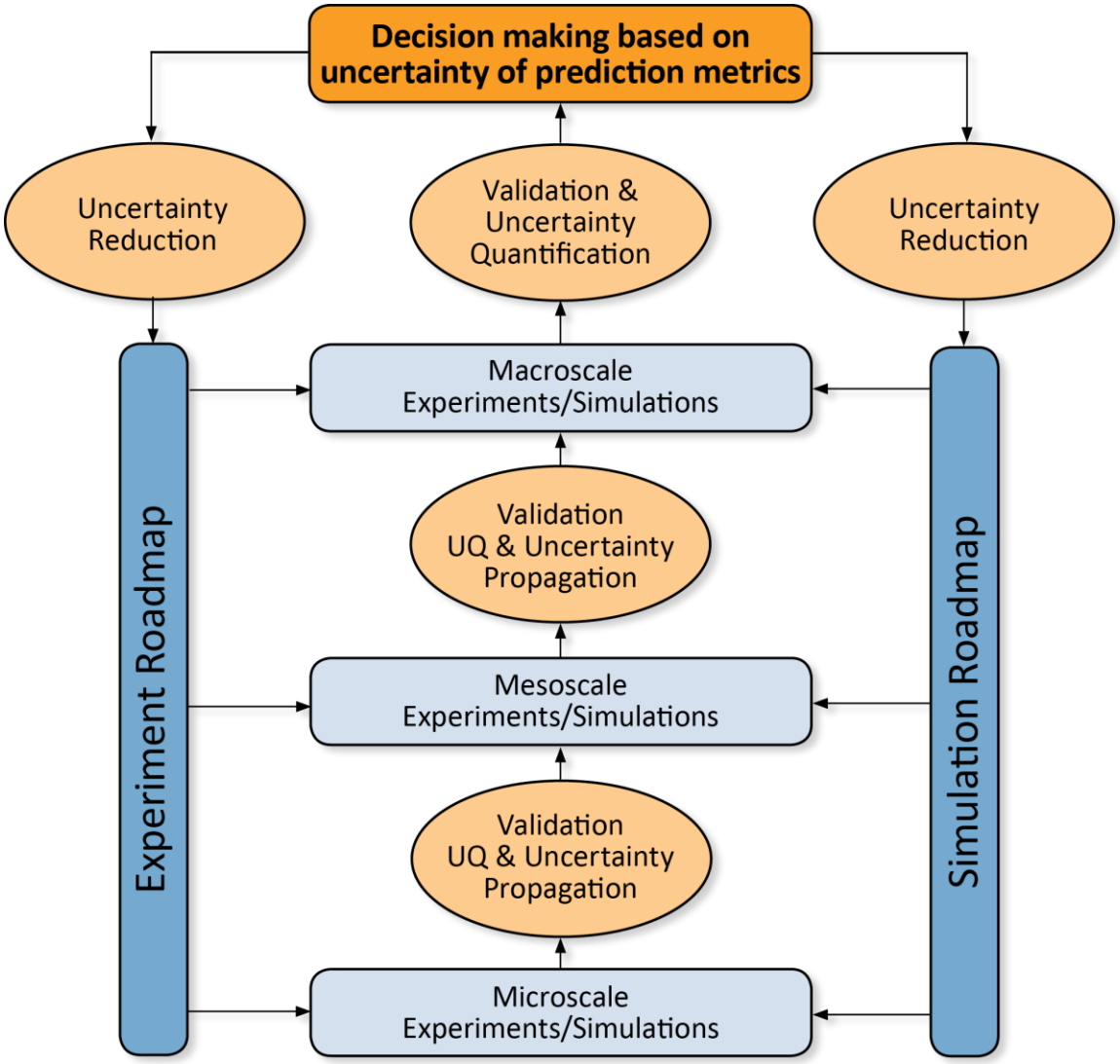


- Exploration of Exascale devices, nodes, and systems, represented by fabrics of interconnected **Architecture BEOs** (behavioral emulation objects)
  - **MICRO: study and characterization of *devices* for Exascale**
    - Fabric of BEOs representing key resources at *device scale*
    - Processor cores, memory hierarchy, chip-level interconnect, I/O
  - **MESO: study and characterization of *nodes* for Exascale**
    - Fabric of BEOs representing key resources at *node scale*
    - Processor devices, memory, server-level interconnect, storage
  - **MACRO: study and characterization of *systems* for Exascale**
    - Fabric of BEOs representing key resources at *system scale*
    - Processing nodes, system-level interconnect, storage
- Architecture BEOs stimulated by corresponding set of **Application BEOs**

Uncertainty Budget – Backbone of CCMT

- Periodic experiments and simulations of *"Demonstration Problem"* essential to establish uncertainty deficit
- We will determine contributions of models to uncertainty of demonstration problem
  - Multiscale uncertainty propagation with Bayesian updating and successive surrogates
  - Physics-inspired surrogate modeling for up-scaling
- Prioritize based on potential for reducing uncertainty
  - Improvements in physical models
  - Improvements in numerics and simulation roadmap
  - Improvements in experimental procedure/measurements
- Essential for achieving accuracy targets here and at NNSA

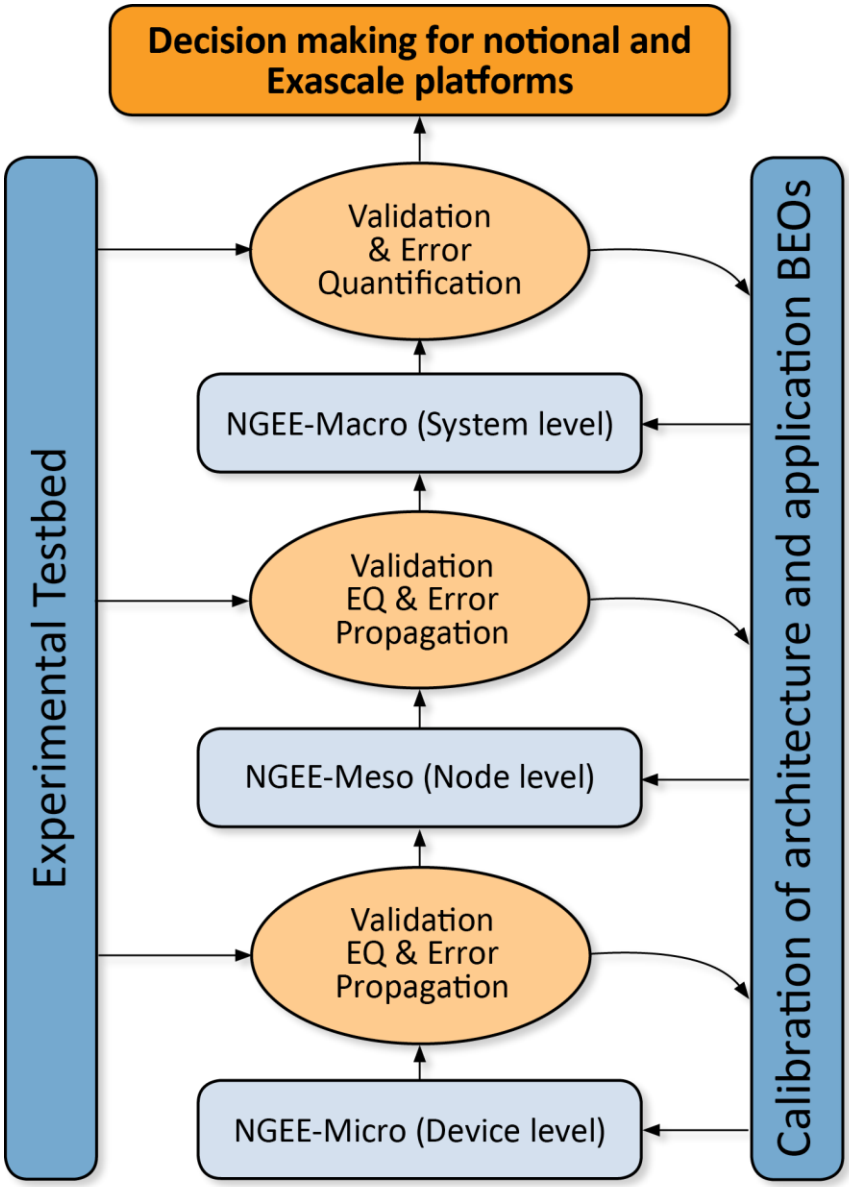
Decision Making with Uncertainty Budget



Uncertainty Budget – Implementation

- A dedicated research staff will be in charge of doing the overall uncertainty budget
- Will be assisted by a graduate student
- Will closely interact and obtain uncertainty information from other research staff and students
- Uncertainty budget will be used by *Simulation/ Experiments Planning & Review Team* (SEPRT)
- Uncertainty budget will be used by *Exascale Co-Design Team* (ECT)
- Uncertainty budget will be used by *Center Management Committee* for resource allocation

Exascale Emulation Uncertainty Budget



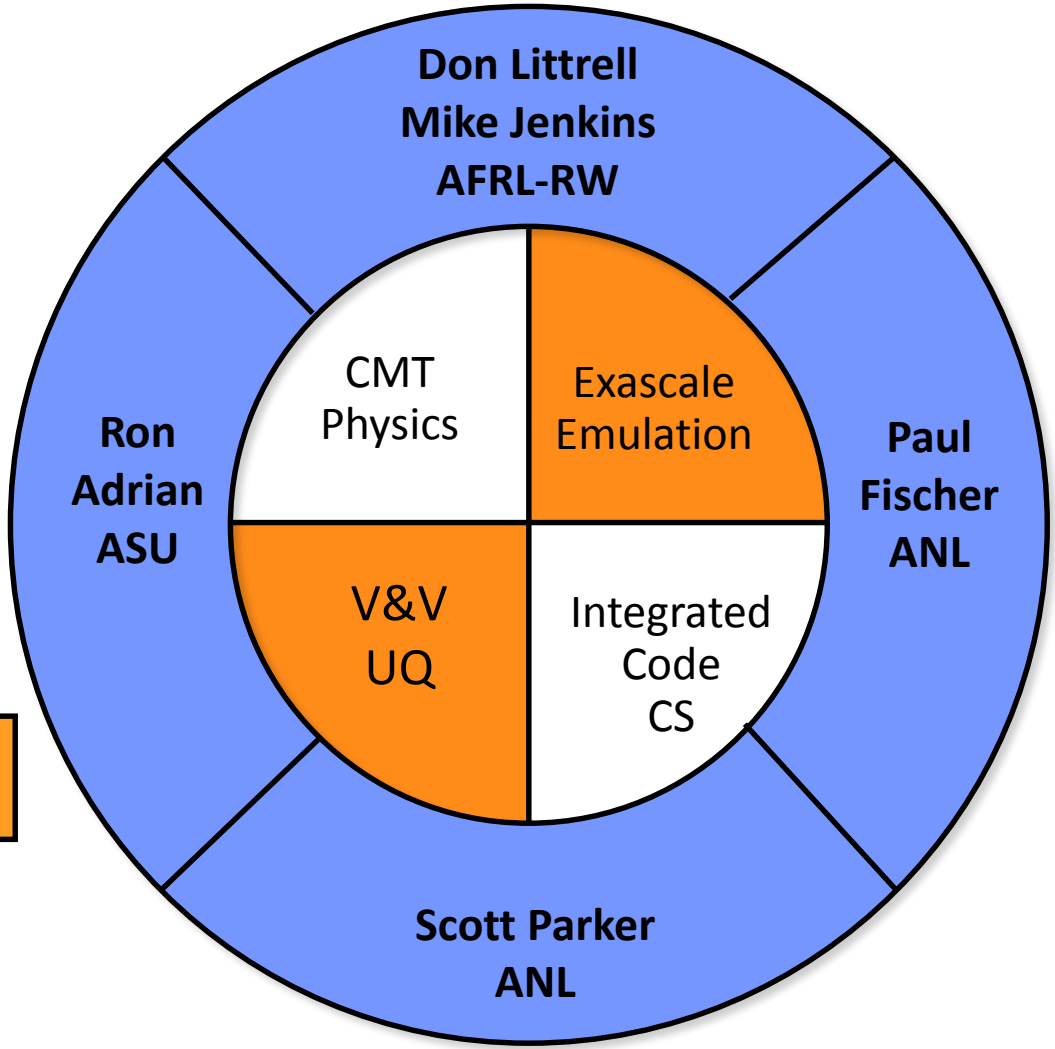
Same cycle for notional and exascale platforms but with uncertainty quantification and propagation

V&V UQ– Unique Aspects

- Uncertainty budget driven decision making
  - Validation that each change in models and experimental procedure improves prediction capabilities
- Pushing parallels between CMT multiscale modeling and multi-level exascale emulation
- Advanced techniques for reducing cost of uncertainty propagation
  - Hybrid surrogates and multiple surrogates.
- Novel techniques for extreme quantities and rare events
- Cross-cutting team-based approach to V&V and UQ

UF Team & Partnership

Explosive experiments, 7 Years, FIRE



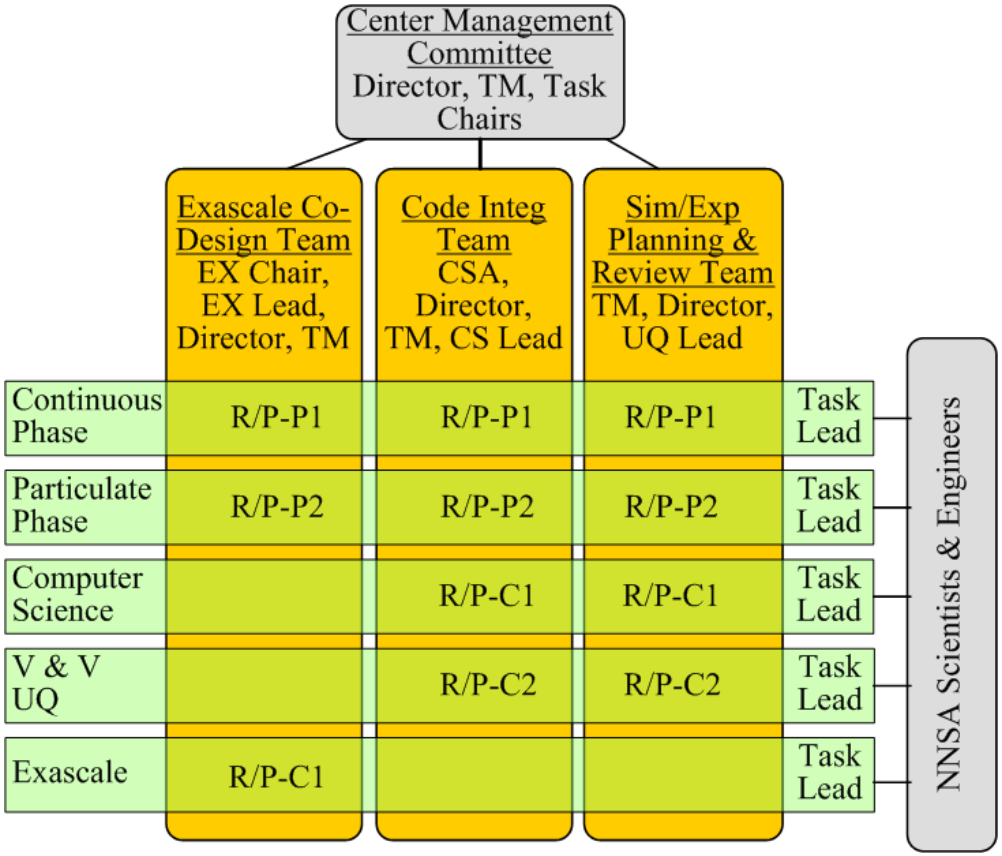
Father of PIV
25 Years
23 Joint publications

Author of Nek
12 Years
9 Joint publications

Subcontract only to ASU

Petascale, 18 Years, 6 Joint publications

Tasks and Teams



The Center will be organized by physics-based tasks and cross-cutting teams, rather than by faculty and their research groups.

NNSA Interaction Goals

Research Exchange

- Maintain center's focus on areas of relevance to NNSA and avoid duplication
- Leverage ongoing cutting-edge research at Labs
  - Experimental data for validation
  - Exascale emulation and simulation, proxy-apps

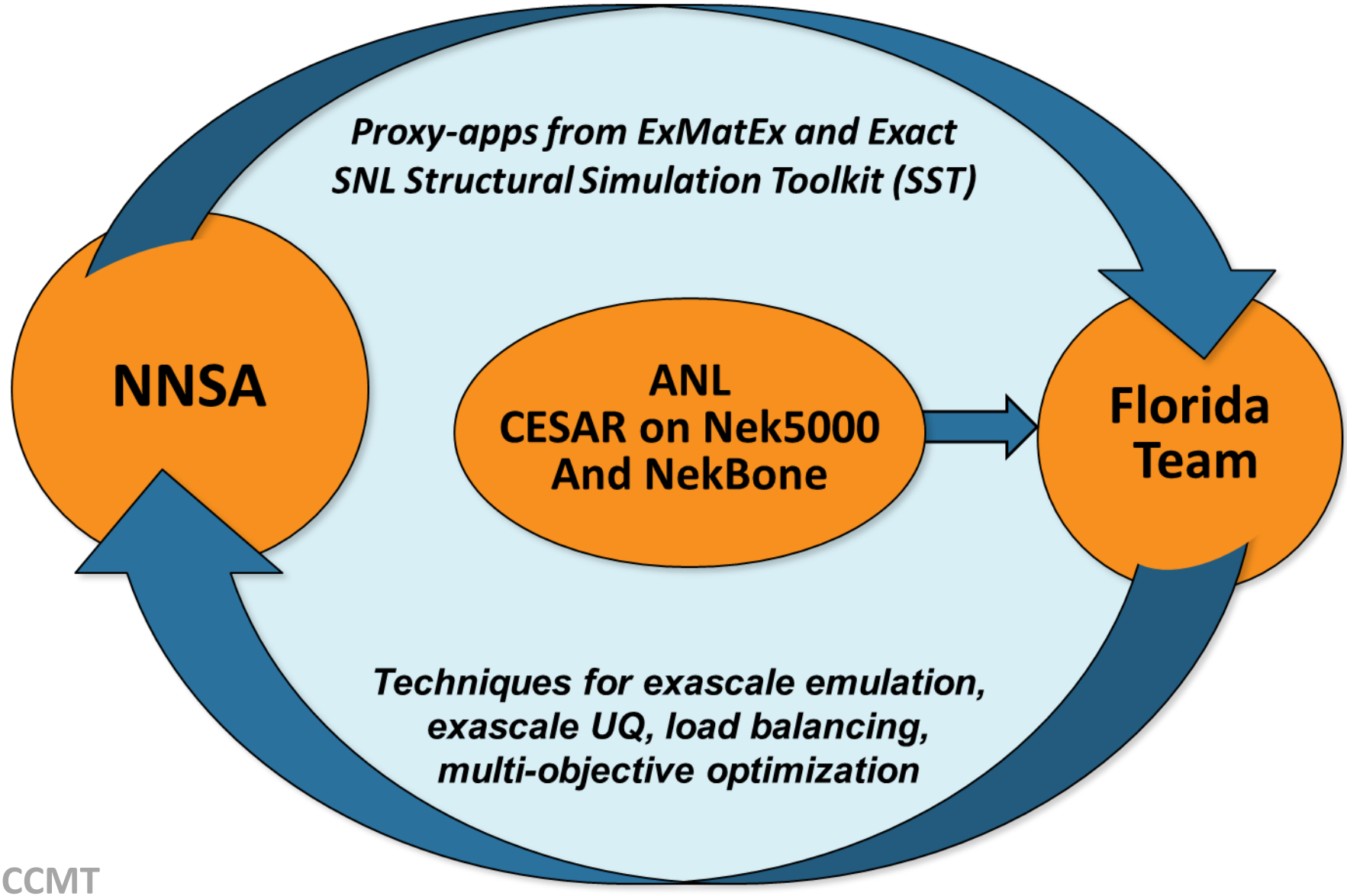
Relationships and Feedback

- Emphasize staff/student interaction with NNSA
  - Facilitate future employment at NNSA labs
  - Nurture existing and build new relationships

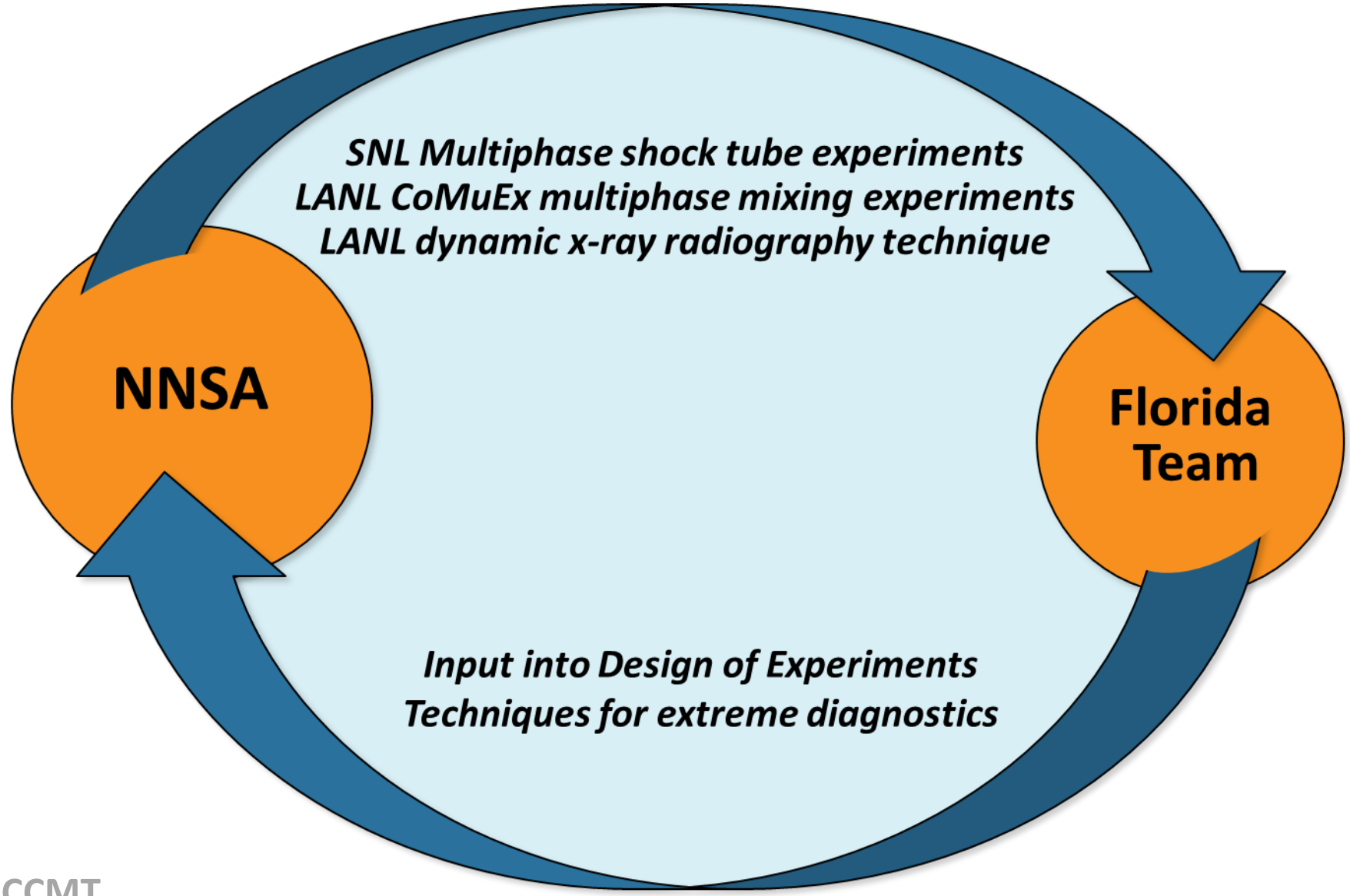
New Curriculum

- Graduate Certificate in "Scientific Computing"
  - PSAAP-II main beneficiary

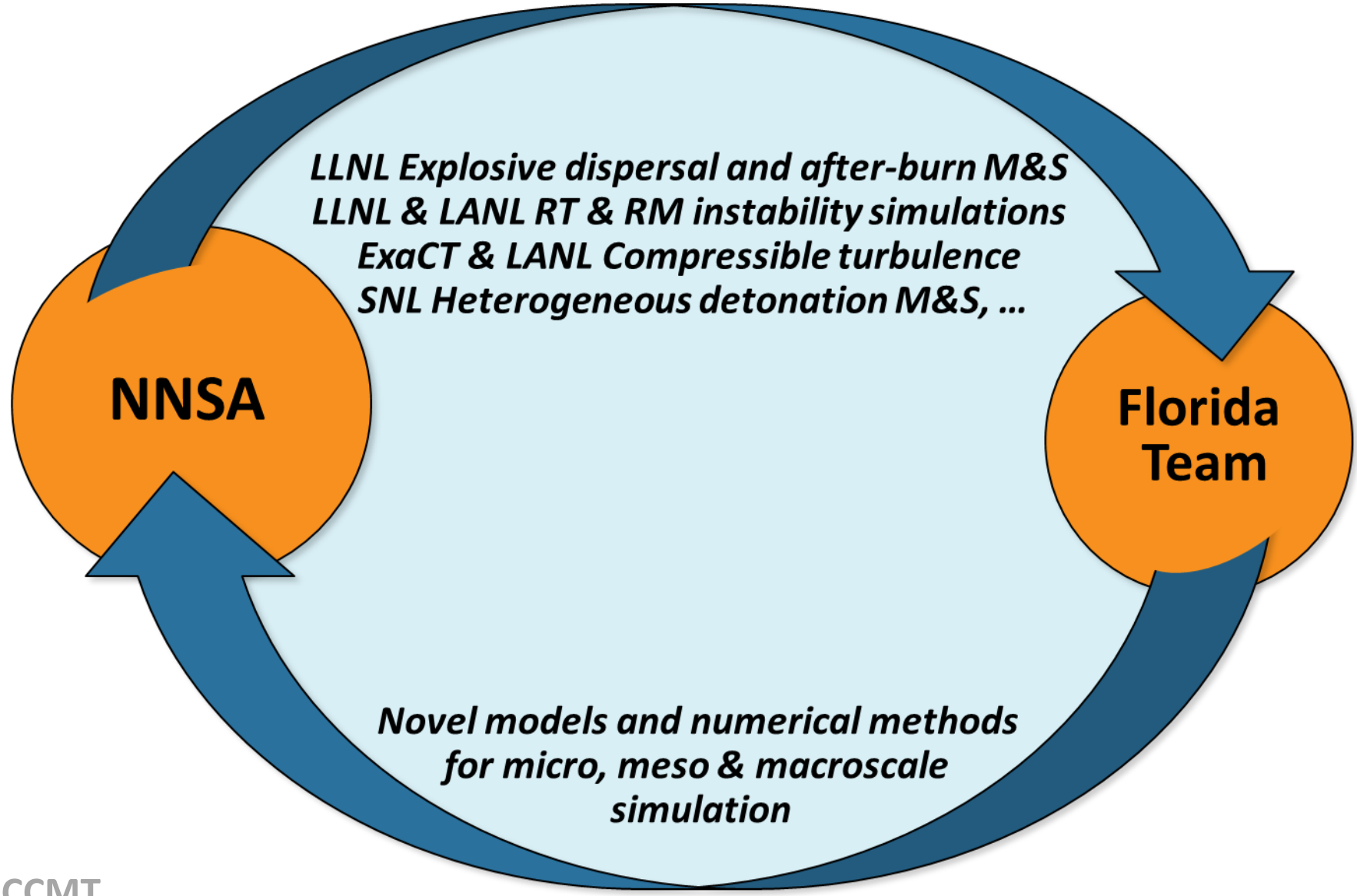
Exascale Interactions



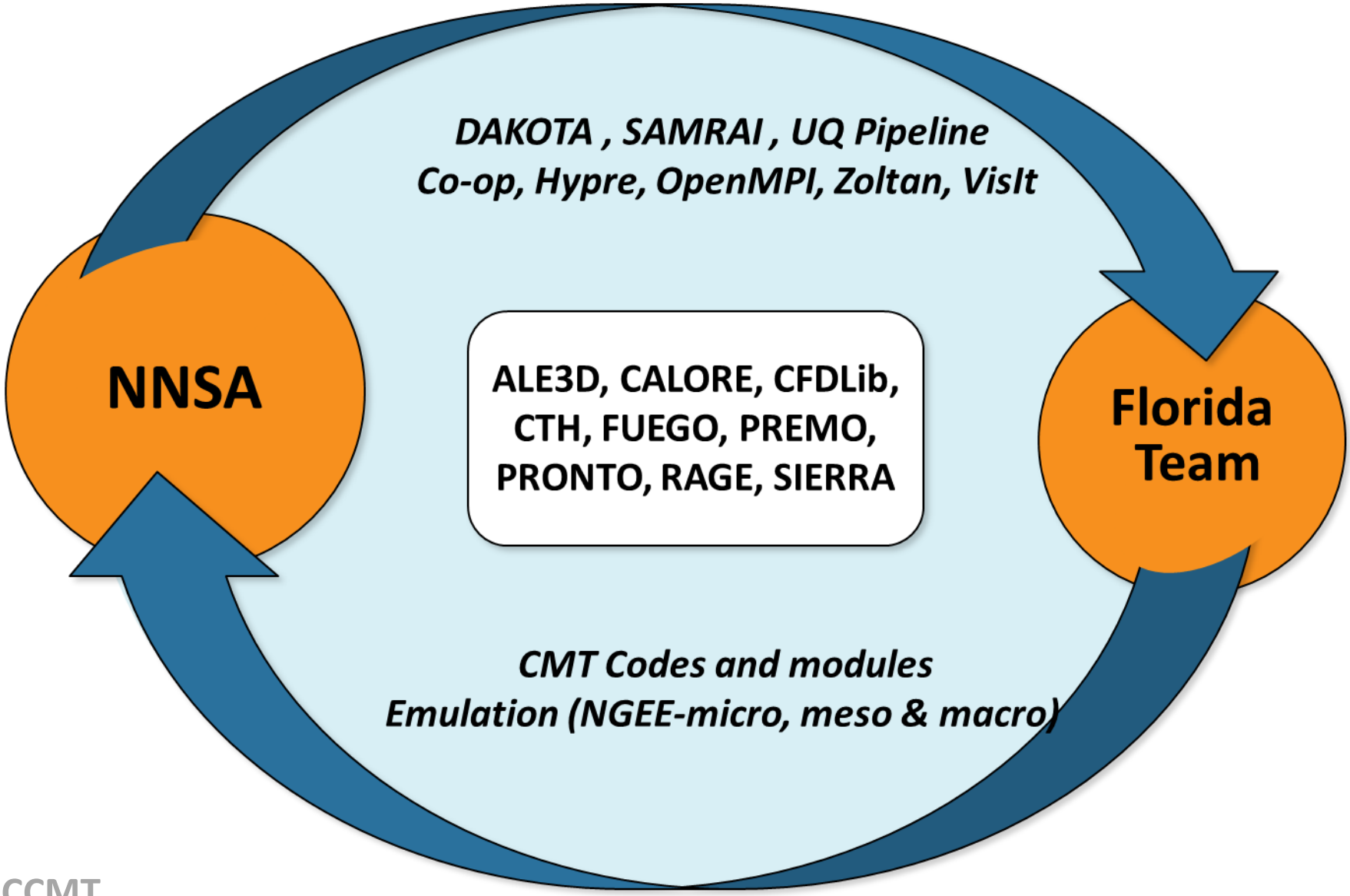
Experimental Interactions



CMT Physics Interactions



Software Interactions

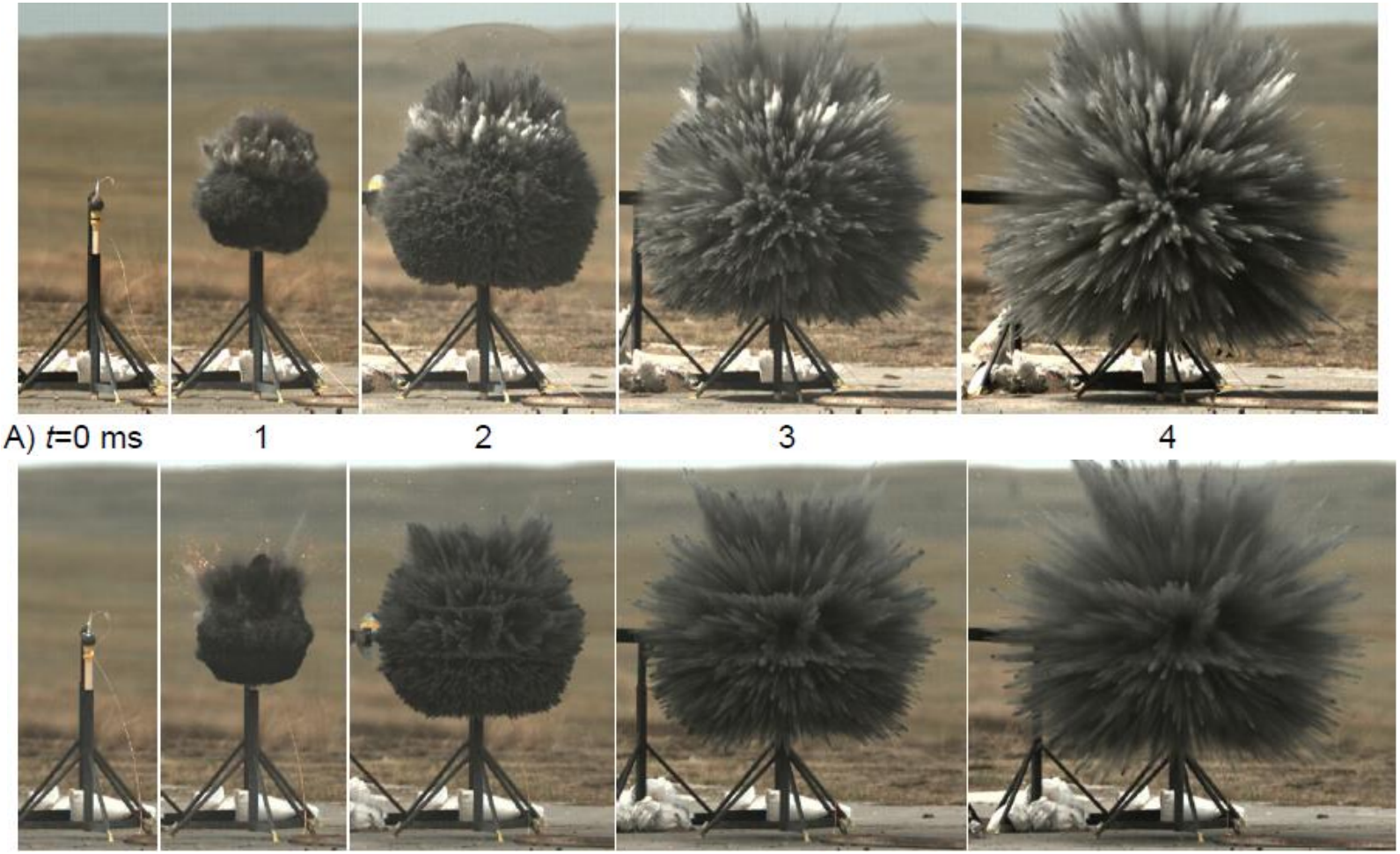


Summary

- Compressible multiphase turbulence (CMT) is a science problem of strong relevance to NNSA
- We have developed a unique multiscale approach to answer important scientific questions
- Innovations in exascale emulation and UQ techniques will enable predictive exascale simulations of CMT
- We have assembled an outstanding team
- We look forward to close interaction with NNSA Labs

Do you have any questions?

Explosive Spherical Dispersion



We desire to perform predictive simulation of these flows with as much multi-scale physics as possible

How Different Pieces Fit